

Fig. 1

E10518_010_HCl_ccorrette
STANDARD 1H OBSERVE

pad=4.5 run with findz0 before acquisition

Archive directory: PC:network places/Share on Grignard/Computers/NMR_DATA
Automation date: autol_04Mar2004

Pulse Sequence: s2pul

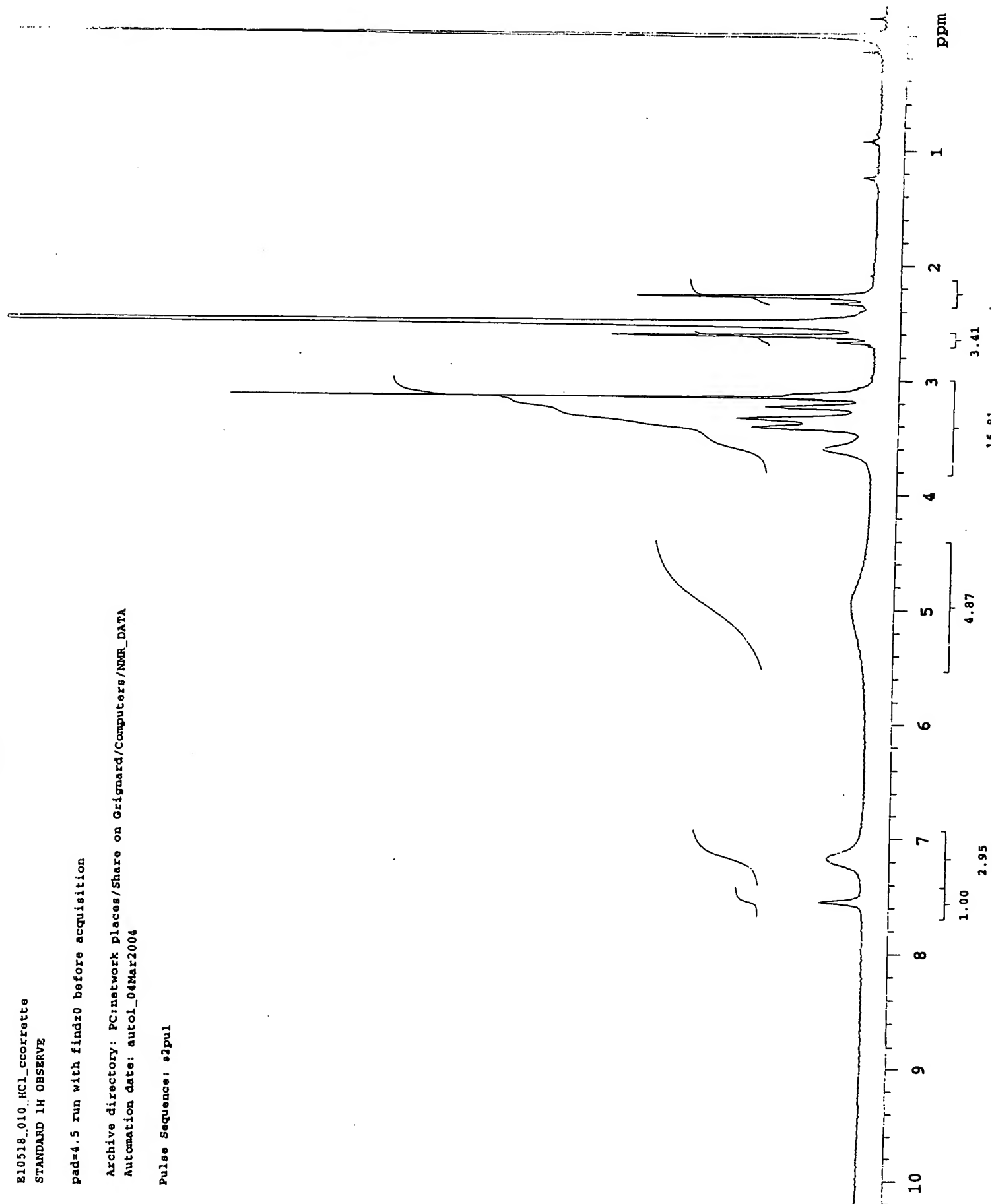
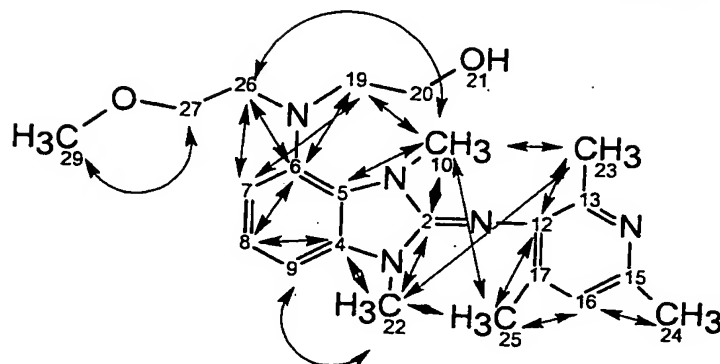


Table-1.: ^1H , ^{13}C -chemical shifts of B10518-10-HCL



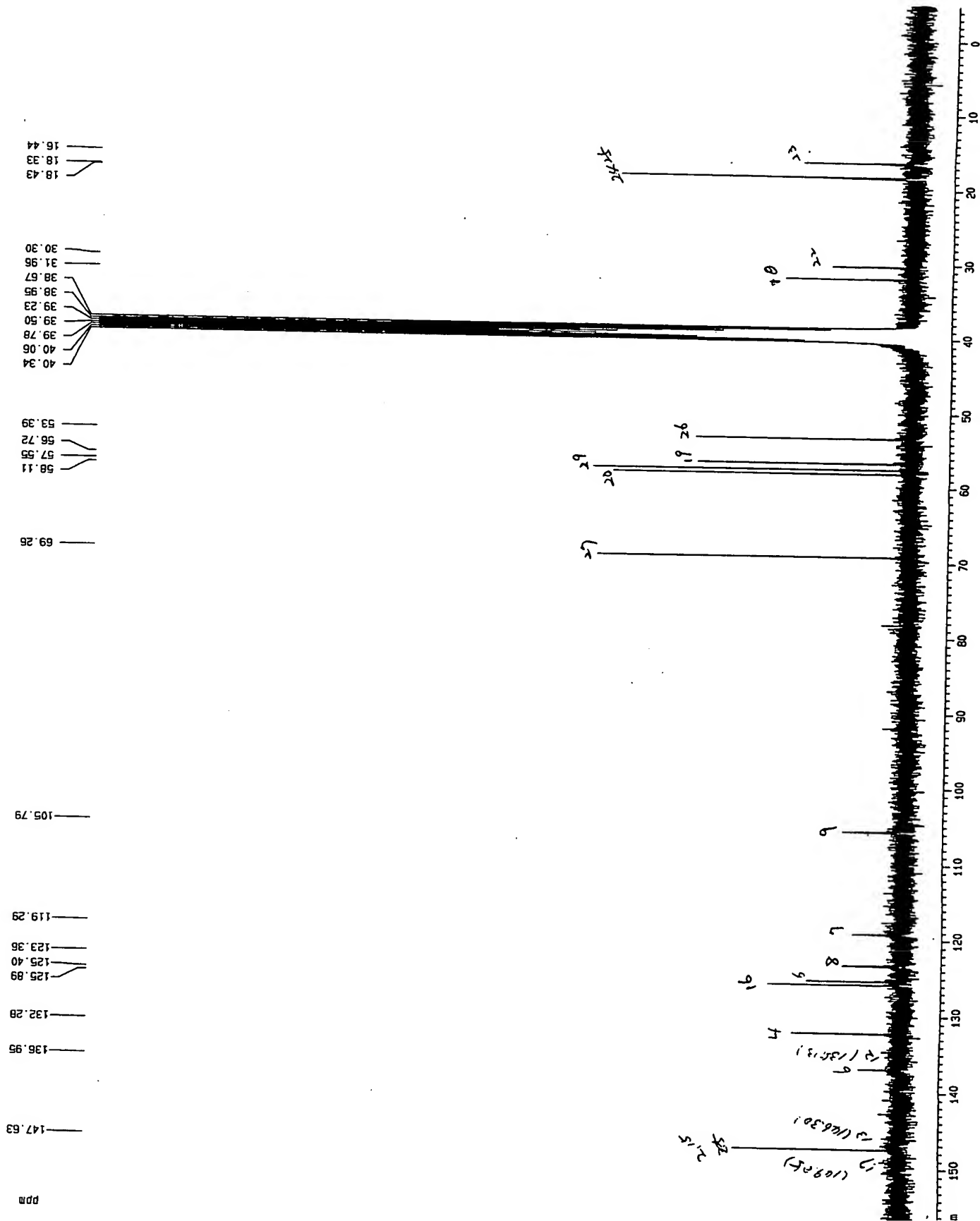
↔ NOE
 → long range coupling

in DMSO at 50°C

	$\delta ^1\text{H}$	multiplicity	J(Hz)	$\delta ^{13}\text{C}$
2-C				*147.63
4-C				132.28
5-C				125.40
6-C				136.95
7-CH	*7.32~7.15			119.29
8-CH	*7.32~7.15			123.36
9-CH	*7.32~7.15			105.79
10-CH ₃	3.706			31.96
12-C				135.13
13-C				146.30
15-C				*147.63
16-CH	7.591	s		125.89
17-C				149.85
19-CH ₂	3.149	m		56.72
20-CH ₂	3.440	m		58.11
22-CH ₃	3.465	s		30.30
23-CH ₃	2.637	s		14.44
24-CH ₃	2.685	s		*218.43
25-CH ₃	2.320	s		*218.33
26-CH ₂	3.249	t	5.9 5.4	53.39
27-CH ₂	3.362	t	5.9 5.4	69.26
29-CH ₃	3.161	s		57.55

*, * 1, * 2 couldn't be assigned due to overlapping of the peaks.

Fig. 2



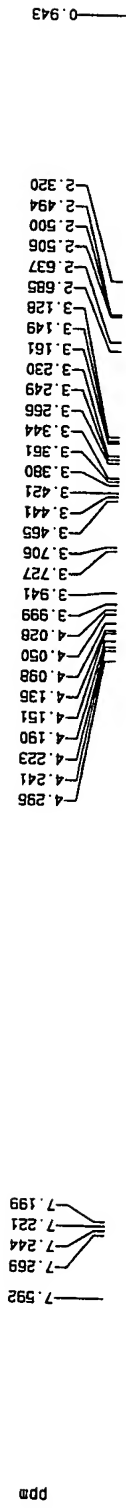
Current Data Parameters
NAME 810518-10-HC1
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040326
Time 1.26
INSTRUM qnp300
PROBHD 5 mm QNP 1H
PULPROG zgpg
TD 65536
SOLVENT CDCl3
NS 6400
DS 4
SWH 16233.767 Hz
FIDRES 0.247708 Hz
AQ 2.0165587 sec
RG 32768
DM 30.800 usec
DE 6.00 usec
TE 300.0 K
d11 0.03000000 sec
d12 0.0002000 sec
PL13 19.00 dB
d1 2.00000000 sec
CPOPRG2 waltz16
PCPD2 100.00 usec
SF02 300.1312005 MHz
NUC2 1H
PL2 120.00 dB
PL12 19.00 dB
P1 3.00 usec
SF01 75.4752658 MHz
NUC1 13C
PL1 -5.00 dB

F2 - Processing parameters
SI 32768
SF 75.4678053 MHz
WDW EM
SSB 0
LB 0.40 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 34.00 cm
F1P 157.856 ppm
F1 11913.04 Hz
F2P -4.900 ppm
F2 -369.78 Hz
PPHCH 4.76653 ppm/cm
HZCH 361.25879 Hz/cm

Fig. 3



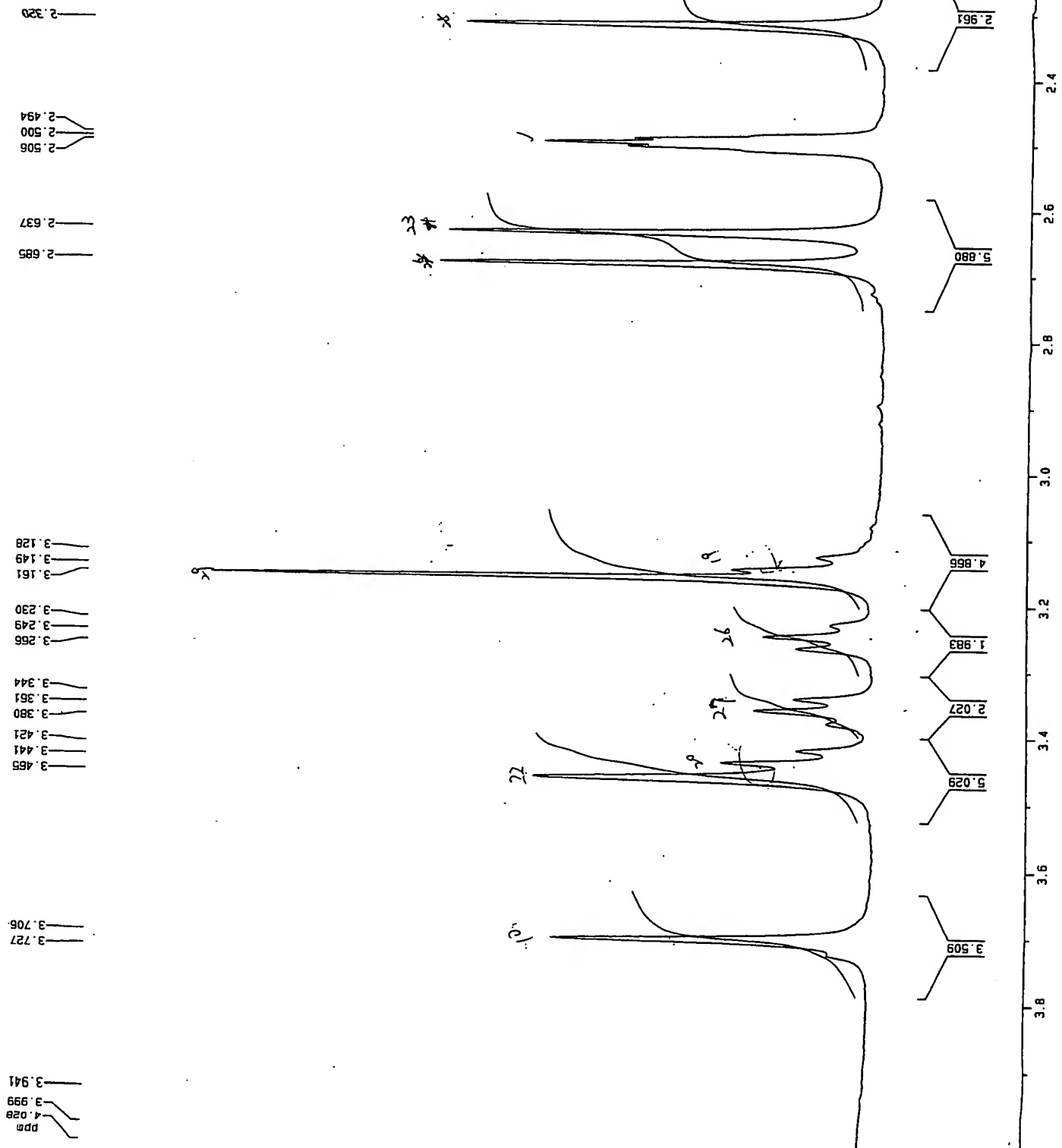
Current Data Parameters
NAME 810518-10-HCl
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040325
Time 12.58
INSTRUM dpx300
PROBHD 5 mm QNP 1H
PULPROG zg0
TD 32768
SOLVENT DMSO
NS 32
DS 4
SHH 2705.628 Hz
FIDRES 0.082559 Hz
AQ 6.0935763 sec
RG 256
DM 184.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
P0 3.00 usec
SFO1 300.1312430 MHz
NUC1 1H
PL1 -5.00 dB

F2 - Processing parameters
SI 16384
SF 300.1300011 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 34.00 cm
FIP 8.645 ppm
F1 2594.76 Hz
F2P -0.369 ppm
F2 -110.87 Hz
PPMCH 0.26514 ppm/cm
HZCH 79.57729 Hz/cm

Fig. 4



Current Data Parameters
NAME 810518-10-HC1
EXPNO 1
PROCNO 1

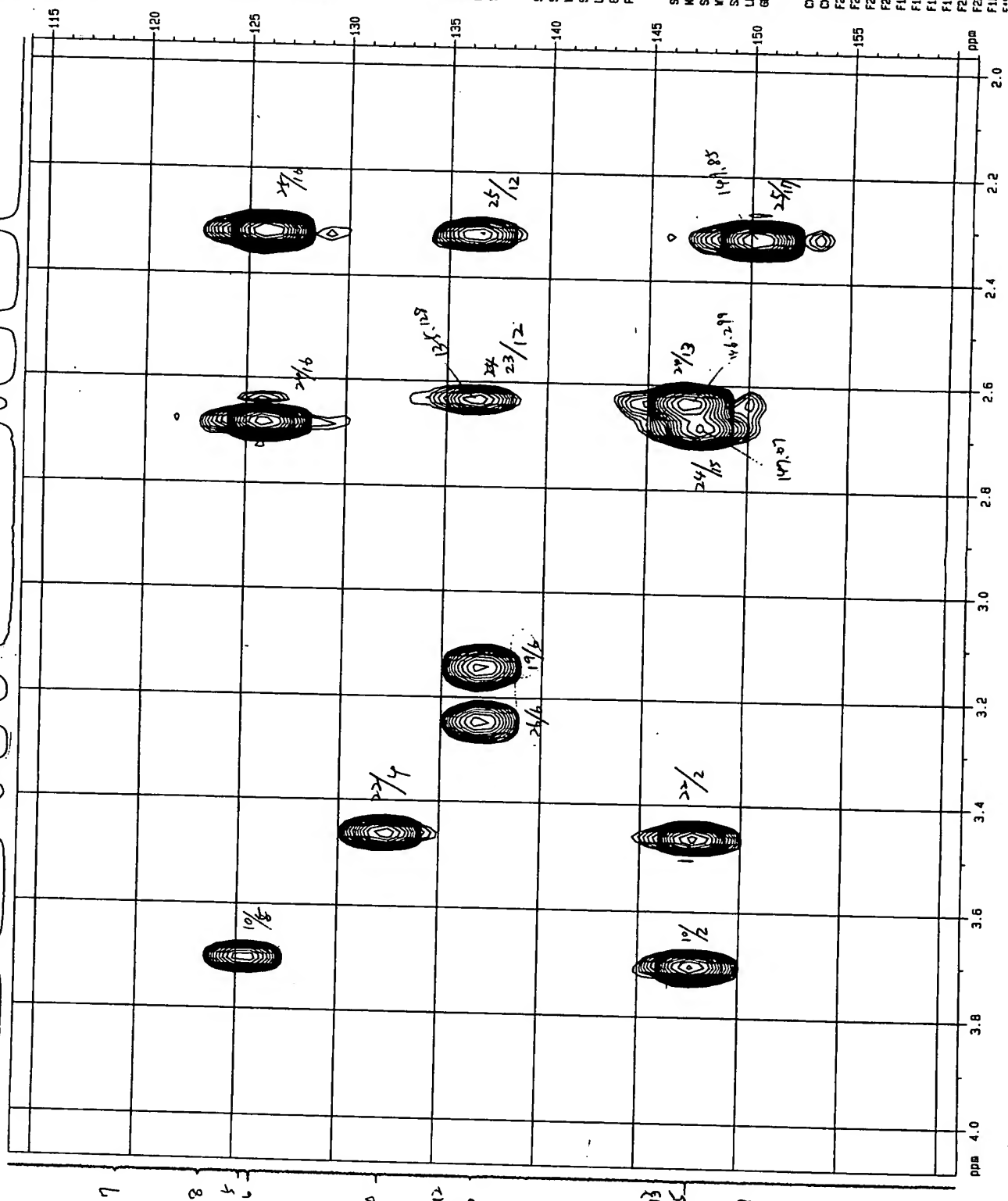
F2 - Acquisition Parameters
Date_ 20040325
Time 12.58
INSTRUM dpx300
PROBHD 5 mm QNP 1H
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 32
DS 4
SWH 2705.628 Hz
FIDRES 0.082569 Hz
AQ 6.0555763 sec
RG 256
DW 184.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
P0 3.00 usec
SF01 300.1312430 MHz
NUC1 1H
PL1 -5.00 dB

F2 - Processing parameters
SI 16384
SF 300.1300011 MHz
WDW EM
SSB 0
LB 0.10 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 34.00 cm
F1P 4.029 ppm
F1 1209.34 Hz
F2P 2.033 ppm
F2 610.18 Hz
PPM0 0.05872 ppm/cm
HZ0 17.62256 Hz/cm

Fig. 5

B10518-10-HC1 in DMSO
HMBC



Current Data Parameters
NAME B10518-10-HC1
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040326
Time 4.00
INSTRUM dm300
PROBHD 5 mm QNP 1H
PULPROG invgprmd
TD 1024
SOLVENT DMSO
NS 56
DS 16
SWH 2705.628 Hz
FIDRES 2.642215 Hz
AQ 0.1892862 sec
RG 32768
DM 184.800 usec
DE 5.00 usec
TE 300.0 K
P1 8.20 usec
P2 16.40 usec
C0 0.0000300 sec
CHST2 145.0000000
d2 0.0034828 sec
d13 0.00000300 sec
d1 2.00000000 sec
SF01 300.1312430 MHz
NUC1 1H
PL1 -5.00 dB
P3 5.80 usec
SF02 75.4752558 MHz
NUC2 13C
PL2 -6.00 dB
D6 0.06000000 sec
P16 1000.00 usec
D16 0.0020000 sec
IN0 0.00003080 sec

F1 - Acquisition Parameters
N00 2
TD 188
SF01 75.47527 MHz
FIDRES 86.346823 Hz
SW 215.087 pps

F2 - Processing parameters
SI 1024
SF 300.1300011 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 256
SF 75.4678052 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 28.00 ca
CX1 22.00 ca
F2XLO 4.085 ppm
F2LO 1226.09 Hz
F2PHI 1.984 ppm
F2PHI 589.31 Hz
F1XLO 161.037 ppm
F1LO 12153.09 Hz
F1PHI 113.982 ppm
F1PHI 8601.95 Hz
F2PHI 0.07577 ppm/ca
F2XCH 22.74192 Hz/ca
F2PHI 2.13686 ppm/ca

Fig. 6

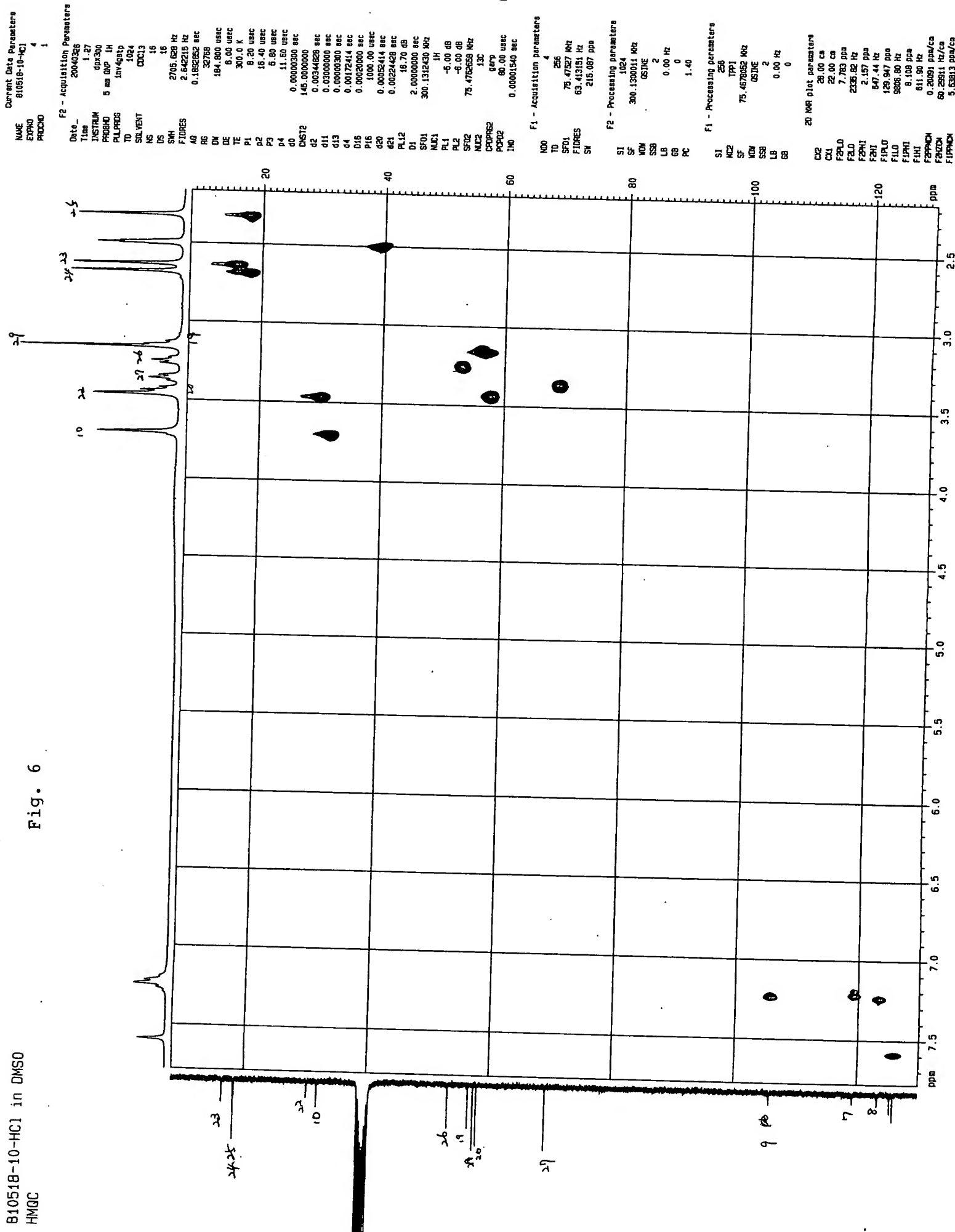


Fig. 7

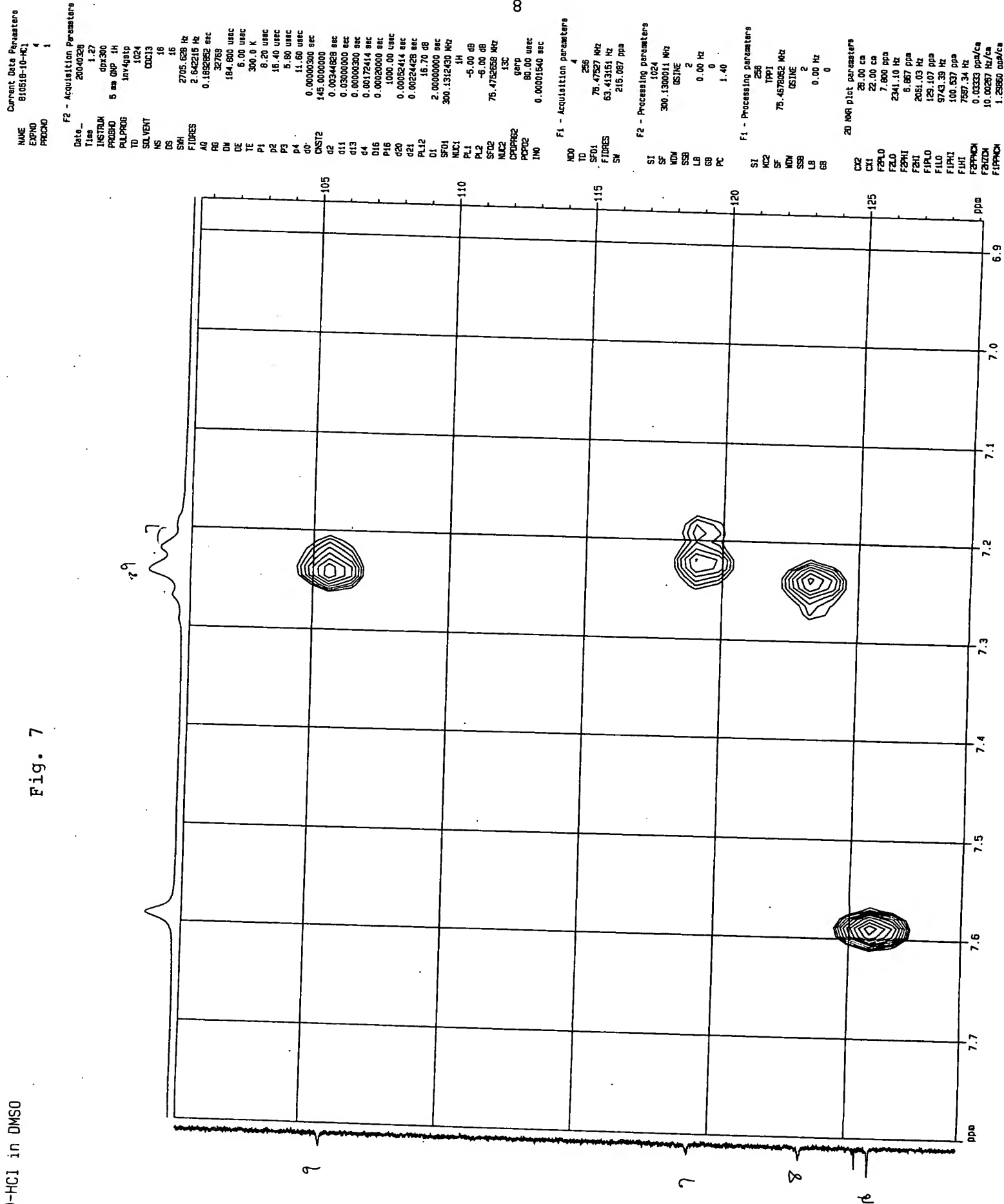
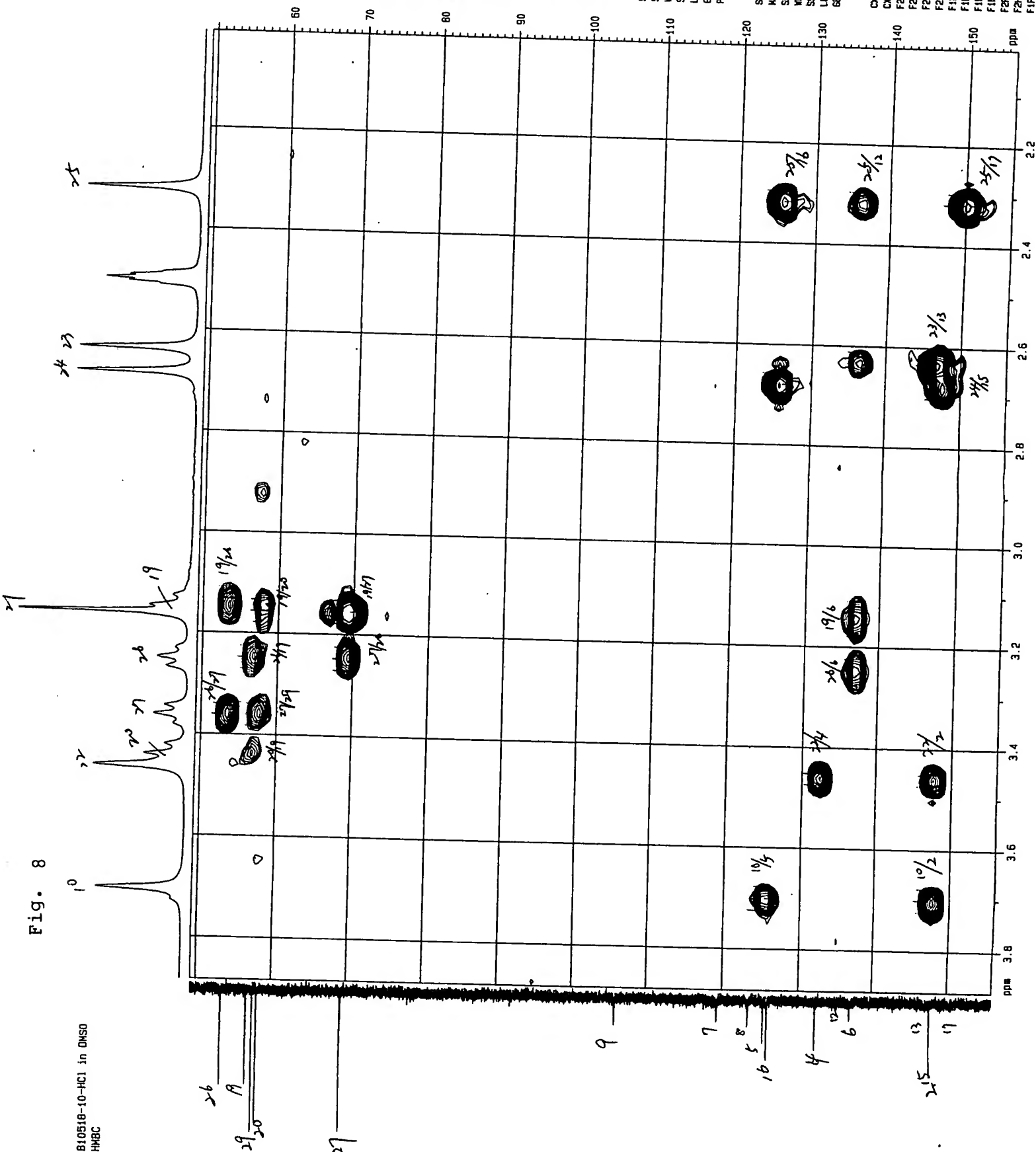


Fig. 8

B10518-10-HCl in DMSO
HMBC



Current Data Parameters
NAME 810518-10-HCl
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040326
Time 4.00
INSTRUM dm300
PROBHD 5 mm QNP 1H
PULPROG invgprind
TD 1024
SOLVENT DMSO
NS 56
DS 16
SWH 2705.628 Hz
FIDRES 2.64215 Hz
AQ 0.1892852 sec
RG 32768
CW 184.800 usec
DE 6.00 usec
TE 300.0 K
P1 8.20 usec
P2 16.40 usec
P3 0.00000000 sec
CNS12 145.0000000
d2 0.00344828 sec
d13 0.00000000 sec
d1 2.00000000 sec
SF01 300.1312430 MHz
NUC1 1H
PL1 -5.00 dB
P3 5.80 usec
SF02 75.4752658 MHz
PL2 13C
D6 -6.00 dB
P16 0.06000000 sec
P16 1000.00 usec
D16 0.00020000 sec
IN0 0.00000000 sec

F1 - Acquisition parameters
NUC0 13C
TD 206
SF01 75.47527 MHz
FIDRES 78.804688 Hz
SN 215.087 ppm

F2 - Processing parameters
SI 1024
SF 300.1300011 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

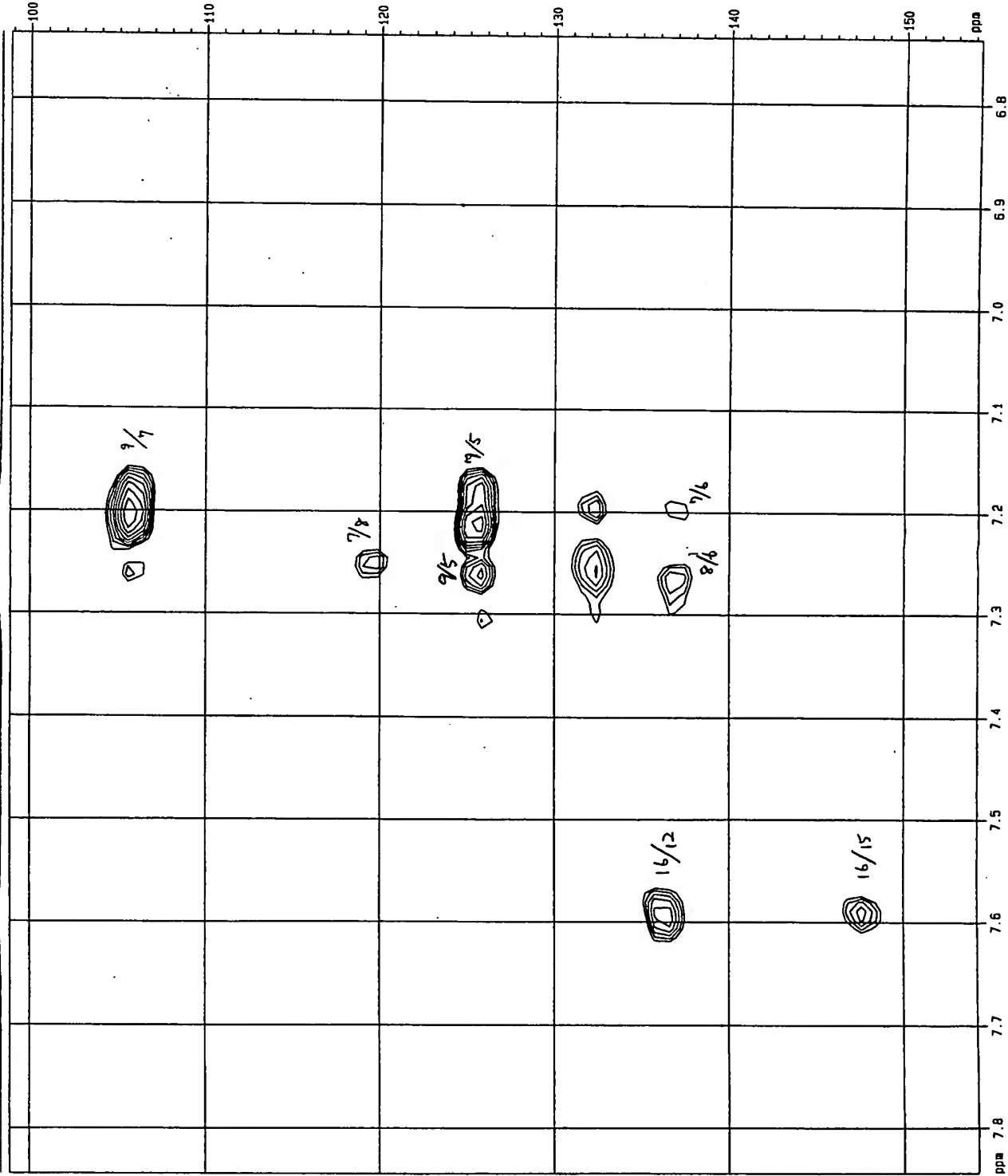
F1 - Processing parameters
SI 255
MC2 OF
SF 75.4678053 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 28.00 cm
CX1 22.00 cm
F2P0 3.883 ppm
F2P1 1165.32 Hz
F2P2 2.008 ppm
F2P3 602.52 Hz
F1P0 155.995 ppm
F1P1 11772.61 Hz
F1P2 49.281 ppm
F1P3 3719.14 Hz
F2P4 0.06597 ppm/cm
F2P5 20.09370 Hz/cm
F2P6 4.80000 Hz/cm

Fig. 9

789

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NAME 810518-10-HC1
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20040326
Time 4.00
INSTRUM cpx300
PROBHD 5 mm QNP 1H
PULPROG invgprind
TO 1024
SOLVENT DMSO
NS 56
DS 16
SWH 2705.628 Hz
FIDRES 2.642215 Hz
AQ 0.1692692 sec
RG 32768
DN 184.800 usec
DE 6.00 usec
TE 300.0 K
P1 8.20 usec
d2 16.40 usec
d0 0.0000300 sec
CNST2 145.0000000
G2 0.00344828 sec
d13 0.0000300 sec
d1 2.0000000 sec
SF01 300.131230 MHz
NUC1 1H
PL1 -5.00 dB
P3 5.80 usec
SF02 75.4752653 MHz
NUC2 13C
PL2 -6.00 dB
GB 0.06000000 sec
P16 1000.00 usec
d16 0.0020000 sec
IN0 0.0000300 sec

F1 - Acquisition Parameters
NU0 2
TD 200
SF01 75.47527 MHz
FIDRES 81.168831 Hz
SW 215.087 ppm

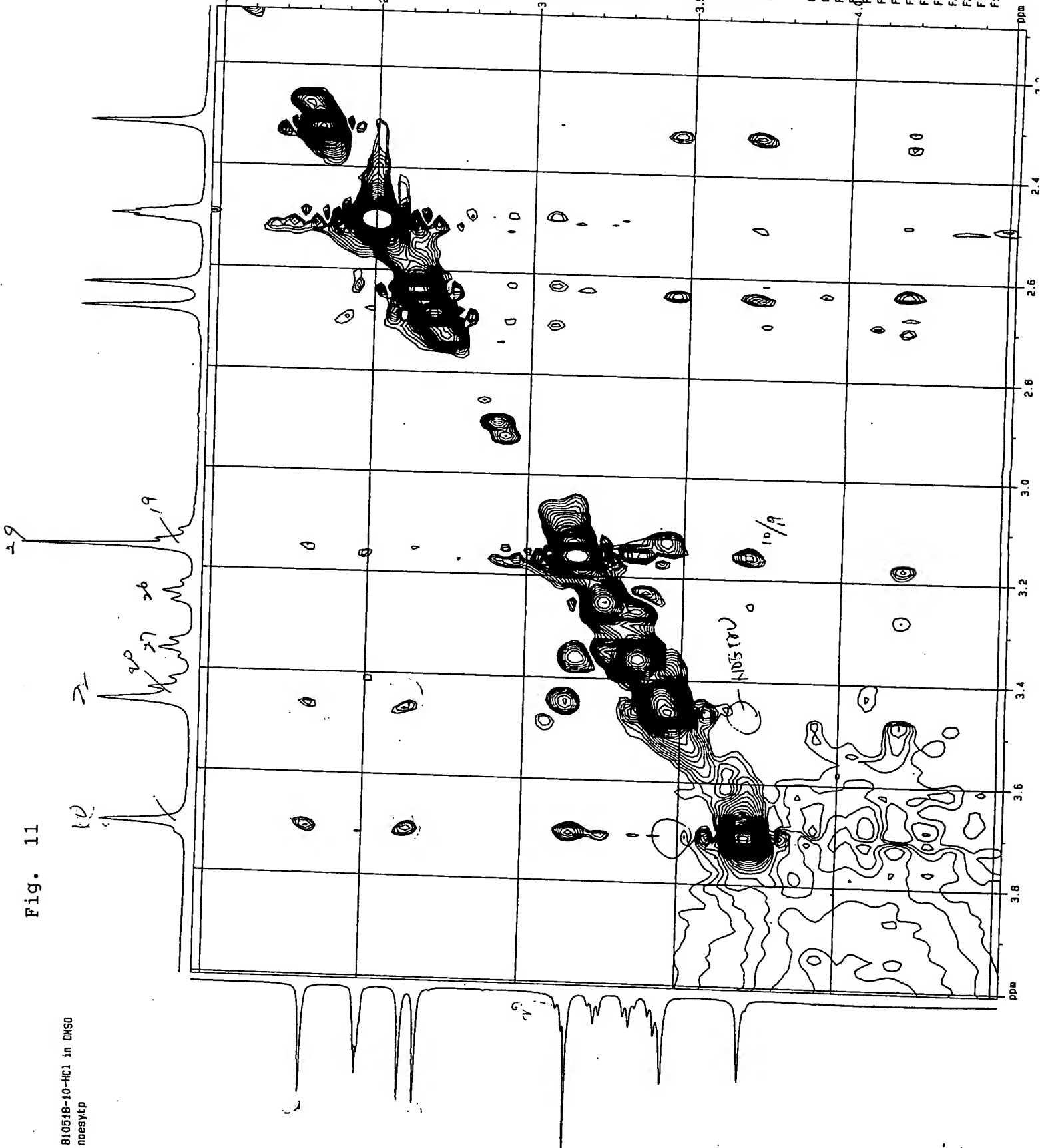
F2 - Processing parameters
SI 1024
SF 300.1300011 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 256
WC2 0
SF 75.4678052 MHz
WDW SINE
SSB 0
LB 0.00 Hz
GB 0

2D NMR plot parameters
CX2 28.00 cm
CX1 22.00 cm
F2P0 7.844 ppm
F2L0 2354.31 Hz
F2PHI 6.735 ppm
F2H1 2021.39 Hz
F1P0 154.319 ppm
F1L0 11645.79 Hz
F1PHI 59.837 ppm
F1H1 7450.52 Hz
F2PPH0 0.03862 ppm/cm
F2PH0 11.8897 Hz/cm
F1PPH0 2.52089 ppm/cm
F1PH0 190.23544 Hz/cm

Fig. 11

810518-10-HC1 in DMSO
noesytp



Current Data Parameters
NAME 810518-10-HC1
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20040325
Time 13.09
INSTRUM dpx300
PROBHD 5 mm QNP 1H
PULPROG noesytp
TD 1024
SOLVENT CDCl3
NS 24
DS 8

2705.628 Hz
2.642215 Hz
0.1892852 sec
256
184.800 usec
6.00 usec
300.0 K
0.00000300 sec
2.00000000 sec
8.20 usec
300.131230 MHz
-5.00 dB
0.80000001 sec
0.00018480 sec

F1 - Acquisition Parameters

ND00 2
TD 256
SF01 300.1312 MHz
FIDRES 10.568858 Hz
SW 9.015 ppm

F2 - Processing parameters

SI 1024
SF 300.1300011 MHz
WDW USINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.00

F1 - Processing parameters

SI 512
TPPI
SF 300.1300011 MHz
WDW USINE
SSB 2
LB 0.00 Hz
GB 0

20 NMR plot parameters

CX2 28.50 cm
CX1 22.00 cm
F2P0 4.006 ppm
F2P1 1202.31 Hz
F2H1 2.087 ppm
F1P0 626.30 Hz
F1L0 4.525 ppm
F1P1 1358.20 Hz
F1H1 1.972 ppm
F2PPHCH 591.96 Hz
F2H2CH 0.06734 ppm/cm
F1PPHCH 20.21062 Hz/cm
F1H2CH 0.11605 ppm/cm
F1H2CH 34.82919 Hz/cm

Fig. 12

